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About the Concept of Molecular Structure

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Abstract
The concept of molecular structure is one of the most important concepts of chemistry. In fact, molecular structure is closely related to the concept of chemical substance and its set of properties, and it is the main factor in the explanation of reactivity. In fact, much of the behavior of substances is explained in terms of the structure of their component molecules. This may explain why people tend to take the notion of molecular structure for granted. However, the problem begins already when it comes to specifying the concept, since there is no clear definition of 'molecular structure' valid for all chemistry. The purpose of the present article is to show that the term 'molecular structure' subsumes very different notions, which depend on how the molecule and its components are conceived, and each of which brings its own difficulties. In particular, we will focus on how the molecule and its structure are devised from a classical view and from a quantum–mechanical view, and will discuss the different problems related with molecular structure that arise in each case.

Keywords Molecular structure · Substances' properties · Systemic concept of molecule · Quantum mechanics · Reductionism

1 Introduction

The concept of molecular structure is one of the most important concepts of chemistry. In fact, molecular structure is closely related to the concept of chemical substance and its set of properties, and it is the main factor in the explanation of reactivity, it is "*the central dogma of molecular science*" (Woolley, 1978, p. 1074). According to Robin Hendry, "*molecular structure is so central to chemical explanation that to explain molecular structure is pretty much to explain the whole of chemistry*" (Hendry,

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2010, p. 183). This claim is due to the fact that much of the behavior of substances is explained in terms of the structure of their component molecules or building groups. This is particularly true in molecular biology, a field in which the structure of the molecules is essential to explain how they interact with one another in living organisms to perform the functions of life. There are even specialized journals on the subject, such as *Journal of Molecular Structure*, devoted to publish structural information on all types of chemical species, both organic and inorganic, in all types of environments, and both in ground and excited states.

This may explain why people tend to take the notion of molecular structure for granted. However, the problem begins already when it comes to specifying the concept, since there is no clear definition of 'molecular structure' valid for all chemistry. Indeed, in the IUPAC Gold book we can find entries for "molecule", "molecular shape", and "structural formula", but there is no entry for "molecular structure".

The purpose of the present article is to show that the term 'molecular structure' subsumes very different notions, which depend on how the molecule and its components are conceived, and each of which brings its own difficulties. In particular, we will focus on how the molecule and its structure are devised from a classical view and from a quantum–mechanical view, and will discuss the different problems related with molecular structure that arise in each case. With this purpose, the article is organized as follows. In Sect. 2, the concept of molecule and its structure is analyzed in molecular chemistry. In this field, the problems refer to how the structure of the molecules of a substance is related with the macroscopic properties of that substance: the idea that molecular structure "explains" the macroscopic chemical level is not free of challenges when considered in detail. Section 3 addresses the concept of molecular structure in the field of quantum chemistry, in which the problems hinge on the conceptual challenges that quantum mechanics imposes on the notion of molecular structure. Finally, in Sect. 4 we will present some final remarks.

2 The Classical View: The Molecule and Its Atomic Components

If one asks a chemist what the components of a molecule are, from a classical viewpoint she will answer that molecules are composed of atoms. In turn, as Hans Primas says, "[t]*he alpha and omega of molecular chemistry is the doctrine that molecules exist as individual objects and that every molecule has a shape*" (Primas, 1994, p. 216). In this context, then, the term 'molecular structure' refers to the spatial arrangement of the atoms in the molecule and the chemical bonds that hold them together. The structural information includes the connectivity of the component atoms, the three-dimensional disposition of atoms in space (which distinguishes between isomers), and the values of bond lengths and dihedral angles. Although assigning a structure to a molecule involves a high degree of idealization, structural information is obtained by various traditional experimental methods, such as spectroscopy and diffraction.

Since the nineteenth century, the chemistry of molecular compounds is a very active scientific field, whose success is based on the synthesis of molecules with new biological or physical properties. It is precisely structural information that enables this creative work. However, this does not mean that, even in this specifically chemical level, the concept of molecular structure is completely free of interpretive difficulties.

were able to confirm the triangular structure that is so straightforwardly obtained within the BOA." (Lang et al., 2024, p. 1760). In turn, much more recently, Lang et al. (2024) propose a "*new definition of molecular structure*" (p. 1761), which is "obtained" by statistical tools on the basis of assuming "*the probabilistic interpretation of quantum mechanics*" (p. 1763). Beyond the fact that it should be discussed whether the probabilistic interpretation involves statistics over non-quantum definite configurations, the authors conclude their work by stressing that "*understanding the emergence of a purely classical structure, e.g., the fact that chiral molecules exist in unique enantiomers showing optical activity, is still an open problem that remains to be solved*." (Lang et al., 2024, p. 1763).

4 Final Remarks

The concept of molecular structure is essential to the chemical explanation of the material world for several reasons.

- This concept allows the different chemical entities to be identified and discriminated at a microscopic level. As we have said, it is a systemic concept that "merges" the constituents into a new entity with its own specific nature. This aspect of the concept of molecular structure is essential to chemistry and cannot be derived from a mechanical description of the molecule, whether classical or quantum. In fact, not even in terms of classical mechanics can the variety of the microscopic world, and the consequent qualitative variety of the macroscopic world, be explained: "*Chemistry might perhaps be said to be the science of the varieties of matter* […]*, but it is far from obvious that the abstract categories effectively deployed within chemistry can be subordinated to those of classical mechanics, those of object and event*" (Laycock, 2023, p. 5).
- Although, as mentioned, there is no direct link between the molecular structure and the properties of the corresponding chemical substance, the concept of molecular structure contributes to the explanation of the properties of the macroscopic chemical substance. In fact, molecular structure endures small perturbations, and this resilience is crucial to identify different chemical species with specific properties, instead of a continuous energy landscape where changes occur in a continuous way.
- Molecular structure, as a systemic concept that transcends the pure aggregate of atoms, allows us to understand the "contextual" character of the atoms in the molecule. It is the feedback of the overall molecular system (with its structure) on the constituent parts that makes the atoms in the molecule specific. Much of the sub-molecular chemical explanation—i.e. that referring to the characteristics of the atoms in the molecule or to the characteristics of the "pieces" of the molecule in the macromolecule—is based on this assumption. Many biochemical explanations appeal to the parts of the macromolecule—such as the active and/or allosteric site of the protein (see Villani, 2020, 2022)—to explain its biological features or its dynamic behavior (Villani, 2023).

In the present paper we have shown that the concept of molecular structure depends on the ontological-descriptive level considered to define it. At each level, the concept involves certain difficulties. However, if such difficulties are examined carefully, it can be seen that they all arise from the attempt to explain concepts of one level by means of concepts of another level. In particular, the attempt is made to fully explain the macroscopic properties

of substances by means of the molecular structure as understood in classical chemistry and, in turn, to explain the latter in terms of quantum mechanics.

What is not usually said is that the requirement that each level must be explained in terms of the corresponding underlying level hides a reductionist assumption according to which the entities of chemistry are, ultimately, nothing more than complex physical entities. From this reductionist perspective, quantum mechanics is the fundamental discipline that should be able to explain in principle all chemistry. As Paul Dirac claimed in his famous dictum: "*The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry [are] completely known from quantum mechanics*" (Dirac, 1929, p. 714).

However, there is nothing that forces us to accept this reductionist assumption, which has been challenged from different perspectives during the last decades. In particular, two different positions deny that the macroscopic properties of substances can be reduced to molecular structure, and that molecular structure can be reduced to quantum mechanics. First, from an emergentist view, the entities and properties of each level emerge from those of the underlying domain but cannot be reduced to them (see, e.g., Hendry, 2010; Matta et al., 2020). Second, from a pluralist view, the ontological priority of the physical world turns out to be a mere metaphysical prejudice: chemical concepts, among them molecular structure, refer to items belonging to the chemical ontology, which only depends on the theory that constitutes it (see: Lombardi & Labarca, 2005, 2006; Lombardi, 2015).

Whichever anti-reductionist alternative is adopted, in both cases it is admitted that molecular structure belongs to the ontology of molecular chemistry, and it can neither be reduced to quantum mechanics nor reduces the macro properties of substances. Here we do not advocate one or the other anti-reductionist perspective. We only want to point out that the anti-reductionist philosophical stance is the most fruitful for chemists in their daily theoretical and experimental practice, since it solves the problems arising from the efforts of reduction.

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